



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 06:04 PM EST

PDB ID : 4L04  
Title : Crystal Structure Analysis of human IDH1 mutants in complex with NADP+ and Ca<sup>2+</sup>/alpha-Ketoglutarate  
Authors : Concha, N.O.; Smallwood, A.M.  
Deposited on : unknown  
Resolution : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

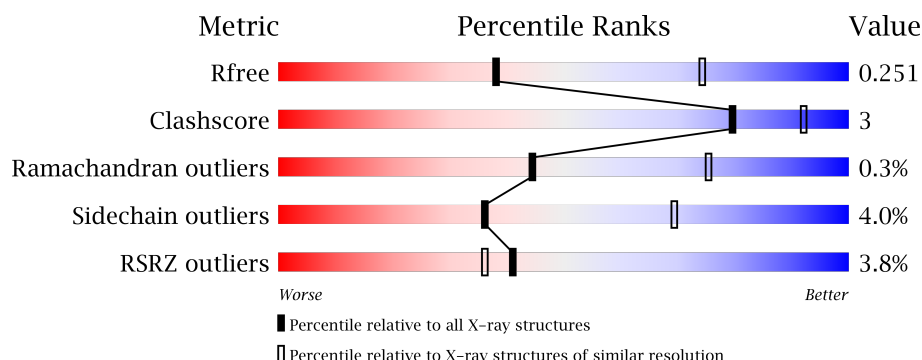
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	425	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>••</div> </div>
1	B	425	<div> <div>%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	C	425	<div> <div>4%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>
1	D	425	<div> <div>5%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
1	E	425	<div> <div>5%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	425	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AKG	C	501	-	-	-	X
2	AKG	D	501	-	-	-	X
2	AKG	E	501	-	-	-	X
2	AKG	F	501	-	-	-	X
3	CA	A	502	-	-	-	X
3	CA	D	502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19647 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3221	2048	546	609	18			
1	B	412	Total	C	N	O	S	0	2	0
			3258	2071	553	616	18			
1	C	412	Total	C	N	O	S	0	0	0
			3206	2030	547	611	18			
1	D	412	Total	C	N	O	S	0	1	0
			3129	1982	535	596	16			
1	E	412	Total	C	N	O	S	0	1	0
			3226	2047	547	614	18			
1	F	412	Total	C	N	O	S	0	1	0
			3184	2025	543	598	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	GLY	CONFLICT	UNP O75874
A	415	SER	-	EXPRESSION TAG	UNP O75874
A	416	LEU	-	EXPRESSION TAG	UNP O75874
A	417	GLU	-	EXPRESSION TAG	UNP O75874
A	418	HIS	-	EXPRESSION TAG	UNP O75874
A	419	HIS	-	EXPRESSION TAG	UNP O75874
A	420	HIS	-	EXPRESSION TAG	UNP O75874
A	421	HIS	-	EXPRESSION TAG	UNP O75874
A	422	HIS	-	EXPRESSION TAG	UNP O75874
A	423	HIS	-	EXPRESSION TAG	UNP O75874
A	424	HIS	-	EXPRESSION TAG	UNP O75874
A	425	HIS	-	EXPRESSION TAG	UNP O75874
B	97	ASN	GLY	CONFLICT	UNP O75874
B	415	SER	-	EXPRESSION TAG	UNP O75874
B	416	LEU	-	EXPRESSION TAG	UNP O75874
B	417	GLU	-	EXPRESSION TAG	UNP O75874
B	418	HIS	-	EXPRESSION TAG	UNP O75874

*Continued on next page...*

*Continued from previous page...*

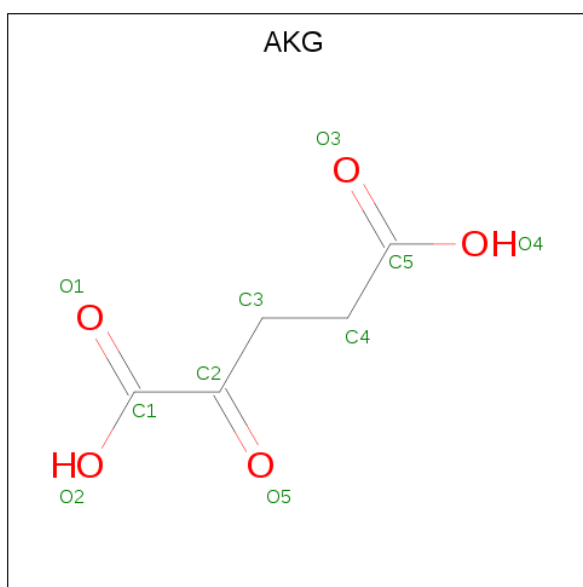
Chain	Residue	Modelled	Actual	Comment	Reference
B	419	HIS	-	EXPRESSION TAG	UNP O75874
B	420	HIS	-	EXPRESSION TAG	UNP O75874
B	421	HIS	-	EXPRESSION TAG	UNP O75874
B	422	HIS	-	EXPRESSION TAG	UNP O75874
B	423	HIS	-	EXPRESSION TAG	UNP O75874
B	424	HIS	-	EXPRESSION TAG	UNP O75874
B	425	HIS	-	EXPRESSION TAG	UNP O75874
C	97	ASN	GLY	CONFLICT	UNP O75874
C	415	SER	-	EXPRESSION TAG	UNP O75874
C	416	LEU	-	EXPRESSION TAG	UNP O75874
C	417	GLU	-	EXPRESSION TAG	UNP O75874
C	418	HIS	-	EXPRESSION TAG	UNP O75874
C	419	HIS	-	EXPRESSION TAG	UNP O75874
C	420	HIS	-	EXPRESSION TAG	UNP O75874
C	421	HIS	-	EXPRESSION TAG	UNP O75874
C	422	HIS	-	EXPRESSION TAG	UNP O75874
C	423	HIS	-	EXPRESSION TAG	UNP O75874
C	424	HIS	-	EXPRESSION TAG	UNP O75874
C	425	HIS	-	EXPRESSION TAG	UNP O75874
D	97	ASN	GLY	CONFLICT	UNP O75874
D	415	SER	-	EXPRESSION TAG	UNP O75874
D	416	LEU	-	EXPRESSION TAG	UNP O75874
D	417	GLU	-	EXPRESSION TAG	UNP O75874
D	418	HIS	-	EXPRESSION TAG	UNP O75874
D	419	HIS	-	EXPRESSION TAG	UNP O75874
D	420	HIS	-	EXPRESSION TAG	UNP O75874
D	421	HIS	-	EXPRESSION TAG	UNP O75874
D	422	HIS	-	EXPRESSION TAG	UNP O75874
D	423	HIS	-	EXPRESSION TAG	UNP O75874
D	424	HIS	-	EXPRESSION TAG	UNP O75874
D	425	HIS	-	EXPRESSION TAG	UNP O75874
E	97	ASN	GLY	CONFLICT	UNP O75874
E	415	SER	-	EXPRESSION TAG	UNP O75874
E	416	LEU	-	EXPRESSION TAG	UNP O75874
E	417	GLU	-	EXPRESSION TAG	UNP O75874
E	418	HIS	-	EXPRESSION TAG	UNP O75874
E	419	HIS	-	EXPRESSION TAG	UNP O75874
E	420	HIS	-	EXPRESSION TAG	UNP O75874
E	421	HIS	-	EXPRESSION TAG	UNP O75874
E	422	HIS	-	EXPRESSION TAG	UNP O75874
E	423	HIS	-	EXPRESSION TAG	UNP O75874
E	424	HIS	-	EXPRESSION TAG	UNP O75874

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	425	HIS	-	EXPRESSION TAG	UNP O75874
F	97	ASN	GLY	CONFLICT	UNP O75874
F	415	SER	-	EXPRESSION TAG	UNP O75874
F	416	LEU	-	EXPRESSION TAG	UNP O75874
F	417	GLU	-	EXPRESSION TAG	UNP O75874
F	418	HIS	-	EXPRESSION TAG	UNP O75874
F	419	HIS	-	EXPRESSION TAG	UNP O75874
F	420	HIS	-	EXPRESSION TAG	UNP O75874
F	421	HIS	-	EXPRESSION TAG	UNP O75874
F	422	HIS	-	EXPRESSION TAG	UNP O75874
F	423	HIS	-	EXPRESSION TAG	UNP O75874
F	424	HIS	-	EXPRESSION TAG	UNP O75874
F	425	HIS	-	EXPRESSION TAG	UNP O75874

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	E	1	Total	C	O	0	0
			10	5	5		

Continued on next page...

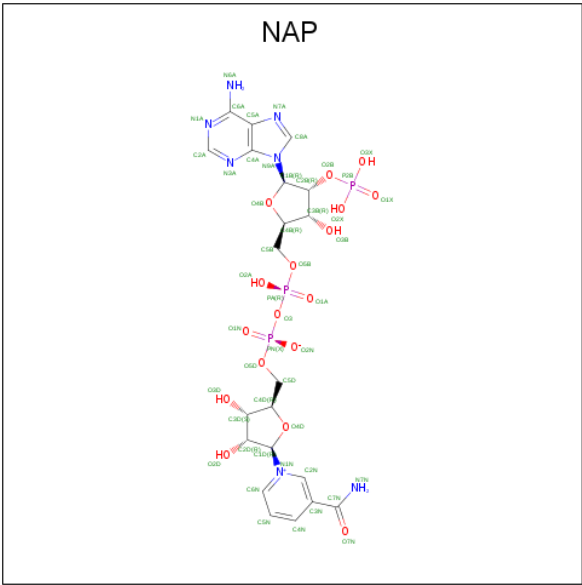
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

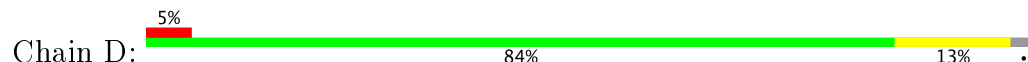
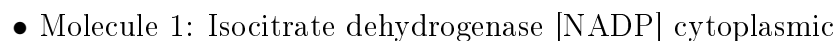
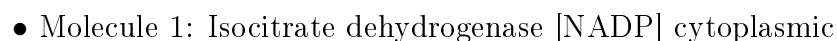
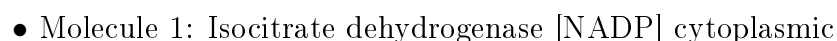
- Molecule 5 is water.

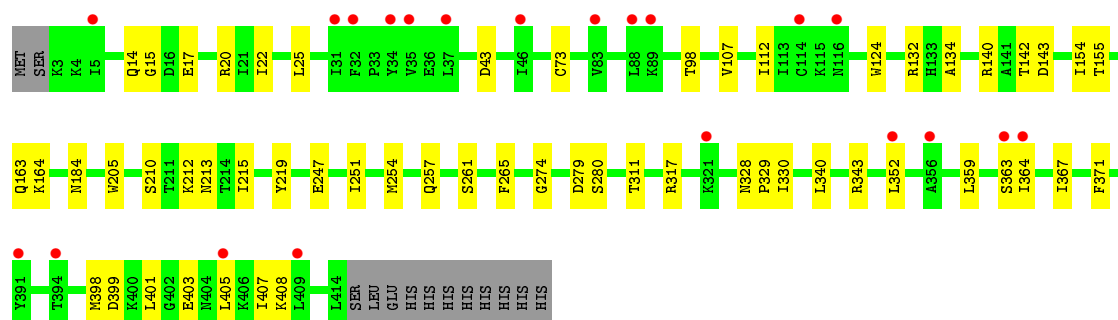
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	13	Total	O	0	0
			13	13		
5	C	16	Total	O	0	0
			16	16		
5	D	8	Total	O	0	0
			8	8		
5	E	7	Total	O	0	0
			7	7		
5	F	7	Total	O	0	0
			7	7		



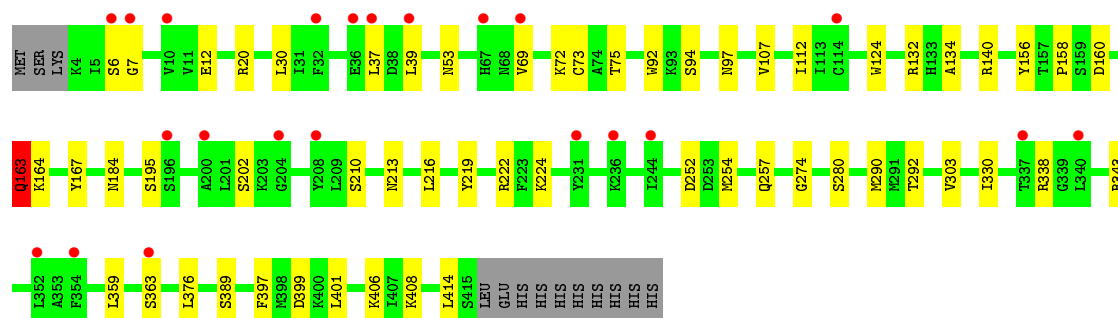
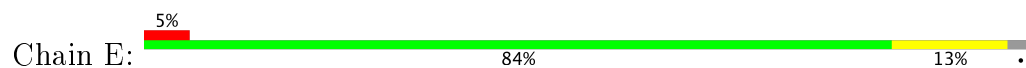


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

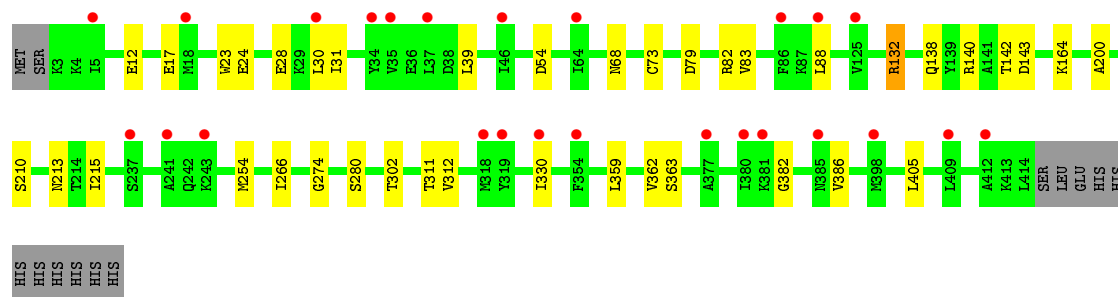
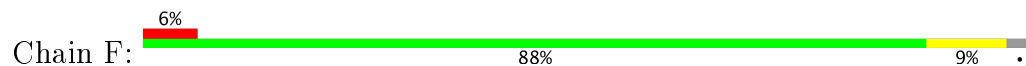




- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.41Å 116.62Å 275.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 2.87 49.24 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.24-2.87) 98.0 (49.24-2.87)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.86Å)	Xtriage
Refinement program	PHENIX, BUSTER 2.11.5	Depositor
R, $R_{free}$	0.200 , 0.259 0.193 , 0.251	Depositor DCC
$R_{free}$ test set	3573 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6255e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, AKG, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	0/3289	0.68	0/4446
1	B	0.47	0/3332	0.68	0/4499
1	C	0.47	0/3272	0.68	0/4422
1	D	0.45	0/3197	0.68	0/4336
1	E	0.47	0/3296	0.68	1/4456 (0.0%)
1	F	0.46	0/3255	0.69	0/4406
All	All	0.46	0/19641	0.68	1/26565 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	163	GLN	C-N-CA	5.21	134.72	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3221	0	3144	20	0
1	B	3258	0	3208	23	0
1	C	3206	0	3111	24	0
1	D	3129	0	2959	23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3226	0	3147	25	0
1	F	3184	0	3075	19	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	48	0	25	1	0
4	B	48	0	25	0	0
4	C	48	0	25	1	0
4	D	48	0	25	0	0
4	E	48	0	25	1	0
4	F	48	0	25	0	0
5	A	18	0	0	0	0
5	B	13	0	0	0	0
5	C	16	0	0	0	0
5	D	8	0	0	0	0
5	E	7	0	0	0	0
5	F	7	0	0	0	0
All	All	19647	0	18818	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:GLN:NE2	1:E:164:LYS:H	1.59	0.99
1:C:19:THR:HG21	1:C:74:ALA:HB3	1.64	0.79
1:E:163:GLN:HA	1:E:163:GLN:OE1	1.90	0.69
1:D:205:TRP:HB3	1:D:265:PHE:HA	1.75	0.68
1:A:142:THR:HG21	1:B:167:TYR:HB3	1.80	0.64
1:F:132:ARG:HB2	1:F:274:GLY:HA3	1.80	0.62
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.82	0.62
1:E:69:VAL:HG11	1:E:343:ARG:HD2	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.82	0.61
1:E:112:ILE:HD13	1:E:330:ILE:HG22	1.83	0.61
1:D:17:GLU:HB2	1:D:311:THR:HB	1.82	0.61
1:E:158:PRO:HD2	1:E:163:GLN:O	2.00	0.61
1:A:155:THR:HB	1:A:166:THR:HA	1.82	0.61
1:B:68:ASN:HA	1:B:302:THR:HG23	1.83	0.60
1:E:107:VAL:HG23	1:E:134:ALA:HB2	1.85	0.58
1:A:219:TYR:HB2	1:B:143:ASP:HB2	1.85	0.57
1:D:155[A]:THR:HG21	1:D:164:LYS:HE3	1.86	0.56
1:D:107:VAL:HG23	1:D:134:ALA:HB2	1.87	0.56
1:D:398:MET:HA	1:D:401:LEU:HD12	1.87	0.56
1:C:16:ASP:O	1:C:19:THR:HG22	2.06	0.56
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.87	0.56
1:A:340:LEU:HD22	1:A:352:LEU:HD11	1.88	0.55
1:C:22:ILE:HD11	1:C:327:THR:HB	1.88	0.55
1:C:158:PRO:HG2	1:C:163:GLN:HB2	1.88	0.54
1:E:163:GLN:CD	1:E:164:LYS:H	2.09	0.54
1:D:14:GLN:HB2	1:D:43:ASP:HA	1.89	0.54
1:D:340:LEU:HD22	1:D:352:LEU:HD11	1.90	0.53
1:E:216:LEU:HD21	1:F:138:GLN:HB3	1.90	0.53
1:C:19:THR:HG23	1:C:73:CYS:SG	2.48	0.53
1:E:132:ARG:HG3	1:E:274:GLY:HA3	1.91	0.53
1:C:333:ILE:O	1:C:337:THR:HG23	2.08	0.53
1:A:215:ILE:HG23	1:B:97:ASN:HD21	1.75	0.52
1:B:158:PRO:HD2	1:B:163:GLN:O	2.11	0.51
1:E:97:ASN:HD21	1:F:215:ILE:HD12	1.75	0.51
1:A:256:ALA:O	1:B:283:GLN:HG2	2.11	0.51
1:D:257:GLN:O	1:D:261:SER:HB3	2.11	0.51
1:E:290:MET:HG3	1:E:376:LEU:HD21	1.93	0.51
1:F:17:GLU:HB2	1:F:311:THR:HB	1.93	0.51
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.93	0.50
1:F:24:GLU:O	1:F:28:GLU:HG2	2.12	0.50
1:A:14:GLN:HB2	1:A:43:ASP:HA	1.93	0.50
2:A:501:AKG:H42	4:A:504:NAP:C4N	2.41	0.50
1:D:112:ILE:HD13	1:D:330:ILE:HG22	1.93	0.50
1:D:22:ILE:HG21	1:D:329:PRO:HB3	1.93	0.49
1:B:209:LEU:HD23	1:B:248:HIS:HD2	1.77	0.49
1:D:403:GLU:O	1:D:407:ILE:HG12	2.12	0.49
1:C:112:ILE:HD13	1:C:330:ILE:HG22	1.94	0.49
1:E:7:GLY:HA3	1:E:37:LEU:HD23	1.94	0.49
1:B:141:ALA:HB1	1:B:180:MET:CE	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLY:HA3	1:A:37:LEU:HD23	1.95	0.48
1:E:210:SER:HB3	1:E:254:MET:HG2	1.95	0.48
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.94	0.47
1:E:53:ASN:HA	1:E:92:TRP:CH2	2.50	0.47
1:A:68:ASN:HA	1:A:302:THR:HG23	1.97	0.47
1:B:24:GLU:O	1:B:28:GLU:HG2	2.15	0.47
1:F:132:ARG:CB	1:F:274:GLY:HA3	2.45	0.47
1:C:219:TYR:HB2	1:D:143:ASP:HB2	1.97	0.47
1:A:403:GLU:O	1:A:407:ILE:HG12	2.15	0.47
1:F:68:ASN:O	1:F:302:THR:HA	2.15	0.47
1:A:359:LEU:HD13	1:A:405:LEU:HD22	1.97	0.46
1:F:210:SER:HB3	1:F:254:MET:HG2	1.96	0.46
1:D:210:SER:HB3	1:D:254:MET:HG2	1.97	0.46
1:F:83:VAL:HA	1:F:88:LEU:HD12	1.98	0.46
1:C:317:ARG:HH11	1:C:320:GLN:HE22	1.63	0.46
1:A:154:ILE:HG23	1:A:167:TYR:HB2	1.98	0.46
1:C:412:ALA:C	1:C:414:LEU:H	2.18	0.46
1:A:24:GLU:O	1:A:28:GLU:HB2	2.16	0.45
1:B:210:SER:HA	1:B:249:ARG:O	2.17	0.45
1:F:330:ILE:HD12	1:F:363:SER:HB3	1.97	0.45
1:E:330:ILE:HD12	1:E:363:SER:HB3	1.99	0.45
1:A:143:ASP:HB2	1:B:219:TYR:HB2	1.98	0.45
1:D:132:ARG:HG3	1:D:274:GLY:HA3	2.00	0.44
1:F:200:ALA:HA	1:F:266:ILE:HG13	1.99	0.44
1:E:338:ARG:HA	1:E:338:ARG:HD3	1.80	0.44
1:F:23:TRP:CE3	1:F:73:CYS:HB2	2.53	0.44
1:C:7:GLY:HA3	1:C:37:LEU:HD23	2.00	0.43
1:B:47:GLU:H	1:B:47:GLU:CD	2.22	0.43
1:B:141:ALA:HB1	1:B:180:MET:HE3	2.00	0.43
1:F:30:LEU:HD13	1:F:359:LEU:HD11	2.01	0.43
1:E:12:GLU:HB2	1:E:39:LEU:HD11	2.00	0.43
1:A:124:TRP:HB3	1:A:285:TYR:CE1	2.54	0.43
1:A:210:SER:HA	1:A:249:ARG:O	2.19	0.43
1:C:312:VAL:HG13	4:C:503:NAP:H3B	2.01	0.43
1:B:213:ASN:O	1:B:217:LYS:HA	2.19	0.43
1:D:212:LYS:HG2	1:D:251:ILE:HG22	2.01	0.43
1:D:22:ILE:HA	1:D:25:LEU:HD12	2.00	0.42
1:B:201:LEU:HD23	1:B:244:ILE:HD11	2.00	0.42
1:C:143:ASP:HB2	1:D:219:TYR:HB2	2.01	0.42
1:E:156:TYR:CE2	1:E:158:PRO:HD3	2.53	0.42
1:E:397:PHE:CE2	1:E:401:LEU:HD11	2.54	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ILE:HA	1:D:371:PHE:O	2.20	0.42
1:F:362:VAL:HG21	1:F:405:LEU:HA	2.01	0.42
1:F:359:LEU:HD13	1:F:405:LEU:HD13	2.00	0.42
1:A:283:GLN:HG2	1:B:256:ALA:O	2.19	0.42
1:E:167:TYR:HB3	1:F:142:THR:HG21	2.02	0.42
1:C:123:GLY:O	1:C:262:GLU:HA	2.20	0.41
1:B:57:THR:HG21	1:B:95:PRO:HA	2.02	0.41
1:C:120:LEU:HD12	1:C:283:GLN:O	2.20	0.41
1:C:97:ASN:HD21	1:D:215:ILE:HD12	1.85	0.41
1:D:330:ILE:HD12	1:D:363:SER:HB3	2.01	0.41
1:C:71:VAL:HG11	1:C:336:TRP:HA	2.03	0.41
1:E:72:LYS:HG2	1:E:73:CYS:O	2.20	0.41
1:C:121:VAL:HG11	1:C:124:TRP:CE2	2.56	0.41
1:B:23:TRP:CD1	1:B:27:LYS:HE2	2.55	0.41
1:C:200:ALA:HA	1:C:266:ILE:HG13	2.03	0.41
1:C:30:LEU:O	1:C:355:PHE:HZ	2.03	0.41
1:E:75:THR:O	4:E:503:NAP:H2N	2.21	0.41
1:E:30:LEU:HD22	1:E:359:LEU:HD11	2.03	0.41
1:F:382:GLY:O	1:F:386:VAL:HG23	2.21	0.41
1:C:201:LEU:HD23	1:C:244:ILE:HD11	2.02	0.41
1:C:210:SER:HB3	1:C:254:MET:HG2	2.01	0.41
1:B:126:LYS:O	1:B:263:GLY:HA3	2.21	0.40
1:D:328:ASN:OD1	1:D:330:ILE:HG12	2.21	0.40
1:E:219:TYR:HB2	1:F:143:ASP:HB2	2.02	0.40
1:A:156:TYR:CE1	1:B:146:VAL:HG13	2.56	0.40
1:B:125:VAL:HG22	1:B:262:GLU:HB2	2.03	0.40
1:D:15:GLY:HA3	1:D:73:CYS:SG	2.60	0.40
1:F:79:ASP:H	1:F:82:ARG:HB2	1.87	0.40
1:C:282:ALA:HB2	1:C:291:MET:SD	2.61	0.40
1:D:359:LEU:HD13	1:D:405:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/425 (96%)	389 (95%)	19 (5%)	1 (0%)	51	81
1	B	412/425 (97%)	391 (95%)	19 (5%)	2 (0%)	32	66
1	C	410/425 (96%)	384 (94%)	26 (6%)	0	100	100
1	D	411/425 (97%)	386 (94%)	23 (6%)	2 (0%)	32	66
1	E	411/425 (97%)	389 (95%)	21 (5%)	1 (0%)	51	81
1	F	411/425 (97%)	387 (94%)	22 (5%)	2 (0%)	32	66
All	All	2464/2550 (97%)	2326 (94%)	130 (5%)	8 (0%)	44	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	TRP
1	D	163	GLN
1	E	124	TRP
1	F	164	LYS
1	A	124	TRP
1	B	271	ASN
1	D	124	TRP
1	F	31	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/362 (93%)	326 (97%)	11 (3%)	43	76
1	B	345/362 (95%)	332 (96%)	13 (4%)	38	71
1	C	333/362 (92%)	320 (96%)	13 (4%)	37	70
1	D	312/362 (86%)	297 (95%)	15 (5%)	30	62
1	E	339/362 (94%)	318 (94%)	21 (6%)	21	50
1	F	326/362 (90%)	318 (98%)	8 (2%)	53	82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1992/2172 (92%)	1911 (96%)	81 (4%)	36 68

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	90	GLN
1	A	94	SER
1	A	140	ARG
1	A	155	THR
1	A	160	ASP
1	A	280	SER
1	A	303	VAL
1	A	312	VAL
1	A	332	SER
1	A	394	THR
1	B	12	GLU
1	B	151	LYS
1	B	164	LYS
1	B	184	ASN
1	B	212	LYS
1	B	252	ASP
1	B	304	GLU
1	B	314[A]	ARG
1	B	314[B]	ARG
1	B	325	THR
1	B	388	ARG
1	B	400	LYS
1	B	414	LEU
1	C	20	ARG
1	C	30	LEU
1	C	47	GLU
1	C	140	ARG
1	C	155	THR
1	C	157	THR
1	C	184	ASN
1	C	252	ASP
1	C	280	SER
1	C	326	SER
1	C	332	SER
1	C	338	ARG
1	C	399	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	20	ARG
1	D	98	THR
1	D	140	ARG
1	D	142	THR
1	D	154	ILE
1	D	184	ASN
1	D	213	ASN
1	D	247	GLU
1	D	279	ASP
1	D	280	SER
1	D	317	ARG
1	D	343	ARG
1	D	364	ILE
1	D	399	ASP
1	D	408	LYS
1	E	6	SER
1	E	20	ARG
1	E	94	SER
1	E	140	ARG
1	E	160	ASP
1	E	163	GLN
1	E	184	ASN
1	E	195	SER
1	E	202	SER
1	E	213	ASN
1	E	222	ARG
1	E	224	LYS
1	E	252	ASP
1	E	280	SER
1	E	292	THR
1	E	303	VAL
1	E	389	SER
1	E	399	ASP
1	E	406	LYS
1	E	408	LYS
1	E	414	LEU
1	F	12	GLU
1	F	39	LEU
1	F	54	ASP
1	F	132	ARG
1	F	140	ARG
1	F	213	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	280	SER
1	F	312	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	B	97	ASN
1	B	228	GLN
1	C	96	ASN
1	C	320	GLN
1	E	97	ASN
1	E	163	GLN
1	E	309	HIS
1	F	68	ASN
1	F	96	ASN
1	F	393	ASN
1	F	404	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AKG	A	501	3	3,9,9	0.49	0	4,11,11	0.53	0
4	NAP	A	504	-	44,52,52	1.66	3 (6%)	51,80,80	1.55	2 (3%)
2	AKG	B	501	3	3,9,9	0.36	0	4,11,11	1.37	0
4	NAP	B	502	-	44,52,52	1.55	3 (6%)	51,80,80	1.91	3 (5%)
2	AKG	C	501	3	3,9,9	0.58	0	4,11,11	1.14	1 (25%)
4	NAP	C	503	-	44,52,52	1.72	3 (6%)	51,80,80	1.53	2 (3%)
2	AKG	D	501	3	3,9,9	0.45	0	4,11,11	0.61	0
4	NAP	D	503	-	44,52,52	1.66	3 (6%)	51,80,80	1.65	2 (3%)
2	AKG	E	501	3	3,9,9	0.34	0	4,11,11	1.25	0
4	NAP	E	503	-	44,52,52	1.63	3 (6%)	51,80,80	1.76	5 (9%)
2	AKG	F	501	3	3,9,9	0.23	0	4,11,11	1.51	1 (25%)
4	NAP	F	503	-	44,52,52	1.64	3 (6%)	51,80,80	1.70	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AKG	A	501	3	-	0/3/9/9	0/0/0/0
4	NAP	A	504	-	-	0/27/67/67	0/5/5/5
2	AKG	B	501	3	-	0/3/9/9	0/0/0/0
4	NAP	B	502	-	-	0/27/67/67	0/5/5/5
2	AKG	C	501	3	-	0/3/9/9	0/0/0/0
4	NAP	C	503	-	-	0/27/67/67	0/5/5/5
2	AKG	D	501	3	-	0/3/9/9	0/0/0/0
4	NAP	D	503	-	-	0/27/67/67	0/5/5/5
2	AKG	E	501	3	-	0/3/9/9	0/0/0/0
4	NAP	E	503	-	-	0/27/67/67	0/5/5/5
2	AKG	F	501	3	-	0/3/9/9	0/0/0/0
4	NAP	F	503	-	-	0/27/67/67	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	503	NAP	C2A-N1A	2.67	1.38	1.33
4	D	503	NAP	C2A-N1A	2.68	1.38	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	NAP	C2A-N1A	2.76	1.39	1.33
4	E	503	NAP	C2A-N1A	2.78	1.39	1.33
4	C	503	NAP	C2A-N1A	2.87	1.39	1.33
4	A	504	NAP	C2A-N1A	3.10	1.39	1.33
4	B	502	NAP	C2A-N3A	3.98	1.38	1.32
4	F	503	NAP	C2A-N3A	4.04	1.38	1.32
4	E	503	NAP	C2A-N3A	4.08	1.39	1.32
4	D	503	NAP	C2A-N3A	4.22	1.39	1.32
4	A	504	NAP	C2A-N3A	4.40	1.39	1.32
4	C	503	NAP	C2A-N3A	4.74	1.40	1.32
4	B	502	NAP	O7N-C7N	7.64	1.39	1.24
4	A	504	NAP	O7N-C7N	8.19	1.41	1.24
4	E	503	NAP	O7N-C7N	8.28	1.41	1.24
4	F	503	NAP	O7N-C7N	8.33	1.41	1.24
4	D	503	NAP	O7N-C7N	8.49	1.41	1.24
4	C	503	NAP	O7N-C7N	8.73	1.42	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	NAP	N3A-C2A-N1A	-11.83	118.55	128.86
4	E	503	NAP	N3A-C2A-N1A	-10.70	119.54	128.86
4	F	503	NAP	N3A-C2A-N1A	-10.67	119.57	128.86
4	D	503	NAP	N3A-C2A-N1A	-10.38	119.82	128.86
4	A	504	NAP	N3A-C2A-N1A	-9.48	120.60	128.86
4	C	503	NAP	N3A-C2A-N1A	-8.83	121.17	128.86
4	E	503	NAP	C4A-C5A-N7A	-2.16	107.32	109.41
2	F	501	AKG	C3-C4-C5	-2.14	109.01	112.66
2	C	501	AKG	C3-C4-C5	-2.04	109.18	112.66
4	E	503	NAP	O7N-C7N-N7N	-2.03	119.69	122.58
4	B	502	NAP	C4A-C5A-N7A	-2.01	107.47	109.41
4	E	503	NAP	O4B-C4B-C5B	2.06	116.34	109.40
4	C	503	NAP	C3N-C7N-N7N	2.07	120.13	117.77
4	A	504	NAP	C3N-C7N-N7N	2.31	120.41	117.77
4	F	503	NAP	C3N-C7N-N7N	2.33	120.43	117.77
4	D	503	NAP	C3N-C7N-N7N	2.39	120.50	117.77
4	E	503	NAP	C3N-C7N-N7N	2.90	121.09	117.77
4	B	502	NAP	C3N-C7N-N7N	3.54	121.82	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AKG	1	0
4	A	504	NAP	1	0
4	C	503	NAP	1	0
4	E	503	NAP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	411/425 (96%)	-0.11	7 (1%) 70 69	39, 69, 98, 124	0
1	B	412/425 (96%)	-0.33	3 (0%) 87 86	38, 55, 79, 94	0
1	C	412/425 (96%)	0.01	15 (3%) 43 38	40, 69, 96, 130	0
1	D	412/425 (96%)	0.12	21 (5%) 29 25	40, 83, 116, 147	0
1	E	412/425 (96%)	0.09	22 (5%) 27 23	40, 71, 101, 121	0
1	F	412/425 (96%)	0.20	25 (6%) 22 18	42, 81, 112, 151	0
All	All	2471/2550 (96%)	-0.00	93 (3%) 41 36	38, 70, 105, 151	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	SER	9.0
1	D	35	VAL	6.5
1	F	35	VAL	6.0
1	D	363	SER	5.5
1	E	7	GLY	4.6
1	F	18	MET	4.3
1	D	409	LEU	4.1
1	E	37	LEU	4.0
1	C	409	LEU	3.9
1	F	34	TYR	3.9
1	F	380	ILE	3.8
1	E	196	SER	3.5
1	D	356	ALA	3.4
1	C	6	SER	3.3
1	F	381	LYS	3.3
1	D	352	LEU	3.3
1	F	37	LEU	3.3
1	D	114	CYS	3.2
1	C	236	LYS	3.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	241	ALA	3.2
1	E	10	VAL	3.2
1	E	231	TYR	3.1
1	F	318	MET	3.1
1	A	10	VAL	3.0
1	F	86	PHE	3.0
1	F	5	ILE	3.0
1	F	319	TYR	3.0
1	C	7	GLY	3.0
1	E	204	GLY	3.0
1	F	64	ILE	3.0
1	E	200	ALA	2.9
1	D	5	ILE	2.9
1	D	37	LEU	2.8
1	D	321	LYS	2.8
1	E	363	SER	2.8
1	E	114	CYS	2.8
1	B	5	ILE	2.8
1	A	31	ILE	2.8
1	A	35	VAL	2.8
1	E	337	THR	2.8
1	D	88	LEU	2.8
1	E	352	LEU	2.8
1	B	7	GLY	2.6
1	E	354	PHE	2.6
1	E	36	GLU	2.6
1	F	330	ILE	2.6
1	C	30	LEU	2.5
1	F	377	ALA	2.5
1	C	372	MET	2.5
1	D	394	THR	2.5
1	E	6	SER	2.5
1	F	46	ILE	2.5
1	D	34	TYR	2.5
1	F	385	ASN	2.5
1	F	125	VAL	2.5
1	F	354	PHE	2.5
1	C	398	MET	2.4
1	C	31	ILE	2.4
1	C	230	ILE	2.4
1	C	405	LEU	2.4
1	F	30	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	67	HIS	2.4
1	C	35	VAL	2.4
1	F	398	MET	2.4
1	A	201	LEU	2.3
1	D	31	ILE	2.3
1	D	364	ILE	2.3
1	F	412	ALA	2.3
1	C	226	ILE	2.3
1	D	32	PHE	2.3
1	E	39	LEU	2.3
1	C	415	SER	2.3
1	F	237	SER	2.3
1	D	116	ASN	2.2
1	D	405	LEU	2.2
1	E	340	LEU	2.2
1	D	46	ILE	2.2
1	E	236	LYS	2.2
1	E	32	PHE	2.2
1	D	391	TYR	2.2
1	F	409	LEU	2.2
1	F	243	LYS	2.2
1	C	36	GLU	2.1
1	B	352	LEU	2.1
1	C	229	GLU	2.1
1	E	244	ILE	2.1
1	D	83	VAL	2.1
1	E	69	VAL	2.1
1	F	88	LEU	2.0
1	A	336	TRP	2.0
1	A	190	GLU	2.0
1	E	208	TYR	2.0
1	D	89	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	AKG	C	501	10/10	0.88	0.30	4.10	79,85,88,88	0
2	AKG	E	501	10/10	0.90	0.35	3.71	91,96,98,98	0
2	AKG	F	501	10/10	0.90	0.29	3.37	86,90,99,99	0
3	CA	D	502	1/1	0.98	0.24	2.91	70,70,70,70	0
2	AKG	D	501	10/10	0.92	0.24	2.86	100,101,102,102	0
3	CA	A	502	1/1	0.97	0.24	2.46	70,70,70,70	0
3	CA	C	502	1/1	0.98	0.24	1.40	62,62,62,62	0
2	AKG	A	501	10/10	0.94	0.21	0.95	74,77,79,79	0
3	CA	A	503	1/1	0.99	0.18	0.92	53,53,53,53	0
3	CA	F	502	1/1	0.96	0.20	0.45	74,74,74,74	0
4	NAP	D	503	48/48	0.87	0.21	0.45	98,109,113,114	0
4	NAP	E	503	48/48	0.94	0.20	0.31	54,68,77,79	0
3	CA	E	502	1/1	0.98	0.23	0.17	72,72,72,72	0
4	NAP	F	503	48/48	0.91	0.20	0.10	84,99,103,105	0
4	NAP	C	503	48/48	0.96	0.18	0.05	50,61,74,75	0
4	NAP	B	502	48/48	0.98	0.17	-0.08	44,51,59,62	0
4	NAP	A	504	48/48	0.96	0.16	-0.49	43,59,68,71	0
2	AKG	B	501	10/10	0.95	0.15	-0.51	41,55,58,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.